

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of cis- and trans-1,3-dichloropropene are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of cis- and trans-1,3-dichloropropene are presented in Table 3-2.

TABLE 3-1. Chemical Identity of the Isomers of 1,3-Dichloropropene

Characteristic	cis-1,3-Dichloropropene	trans-1,3-Dichloropropene	cis- and trans- 1,3-Dichloropropene	Reference
Chemical name	cis-1,3-Dichloropropene	trans-1,3-Dichloropropene	1,3-Dichloropropene	Chemline 1989
Synonyms	cis-1,3-Dichloro-1-propene; cis-1,3-dichloropropylene	trans-1,3-Dichloro-1-propene; trans-1,3-dichloropropylene	1,3-Dichloro-1-propene; 1,3-dichloropropylene	Chemline 1989; HSDB 1989
Trade names	No data	No data	Telone [®] ; Telone II [®] (M-3993); Telone C-17 [®] ; DD [®] (Nemafene); DD-92 [®] ; Terr-O-Cide 15-D; Terr-O-Cide 30-D; Terr-O-Gas 57/43T; Vorlex (Trapex, Ditraxex, MENCS, MIC, MITC)	Yang 1986
Chemical formula	C ₃ H ₄ Cl ₂	C ₃ H ₄ Cl ₂	C ₃ H ₄ Cl ₂	Chemline 1989
Chemical structure			Cl-CH ₂ -CH=CH-Cl	
Identification numbers:				
CAS registry	10061-01-5	10061-02-6	542-75-6	Chemline 1989
NIOSH RTECS	UC8325000	UC8320000	UC8310000	SANSS 1989
EPA hazardous waste	No data	No data	No data	
OHM/TADS	8500391	8500392	8500391-2	OHM/TADS 1989
DOT/UN/NA/IMCO shipping	No data	No data	No data	
HSDB	1503	1504	1503-4	HSDB 1989
NCI	No data	No data	No data	

CAS = Chemical Abstracts Service; EPA = Environmental Protection Agency; DOT/UN/NA/IMCOP = Department of Transportation/United Nations/North America/International Maritime Consultative Organization; HSDB = Hazardous Substance Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials Technical Assistance Data Base; RTECS = Registry of Toxic Effects of Chemical Substances; SANSS = Structure and Nomenclature Search System

TABLE 3-2. Physical and Chemical Properties of the Isomers of 1,3-Dichloropene

Property	cis-1,3-Dichloropropene	trans-1,3-Dichloropropene	cis- and trans- 1,3-Dichloropropene	Reference
Molecular weight	110.98	110.98	110.98	Weast et al. 1988
Color	Colorless	Colorless	Colorless	Sax and Lewis 1987
Physical state	Liquid	Liquid	Liquid	Sax and Lewis 1987
Boiling point	104°C at 1 atm	112°C at 1 atm	104°C and 112°C at 1 atm	Weast et al. 1988
Density at 20°C	1.217 g/mL	1.224 g/mL	1.218-1.224 g/mL	Weast et al. 1988
Odor	Chloroform-like	Chloroform-like	Chloroform-like	Windholz et al. 1983
Odor threshold:				
Water	No data	No data	No data	
Air	1 ppm	1 ppm	1 ppm	Verschuieren 1983
Solubility:				
Water at 25°C	2,700 ppm	2,800 ppm	2,700-2,800 ppm	Dilling 1977
Organic solvents	acetone; toluene; octane; ethanol benzene; chloroform	acetone; toluene; octane; ethanol benzene; chloroform	acetone; toluene; octane; ethanol benzene; chloroform	Sax and Lewis 1987; Weast et al. 1988
Partition coefficients:				
Log octanol/water	1.60 (estimated)	1.60 (estimated)	1.60 (estimated)	CLOGP-PCGEMS 1986
Log K _{oc}	1.36	1.41	1.36-1.41	Kenaga 1980
Vapor pressure at 25°C	43 mmHg	34 mmHg	34-43 mmHg	Dilling 1977
Henry's law constant:				
at 20°C	1.2x10 ⁻³ atm-m ³ /mol	8.0x10 ⁻⁴ atm-m ³ /mol	1.2x10 ⁻³ to	Leistra 1970
at 25°C			8.0x10 ⁻⁴ atm-m ³ /mol 3.55x10 ⁻³ atm-m ³ /mol	EPA 1981
Autoignition temperature	No data	No data	No data	
Flashpoint (open cup)	35°C	35°C	35°C	Sax and Lewis 1987
Flammability limits (air)	No data	No data	5.3%-14.5%	OHM/TADS 1989
Conversion factors				
in air (20°C)				
ppm (v/v) to mg/m ³	4.61	4.61	4.61	Verschuieren 1983
mg/m ³ to ppm (v/v)	0.22	0.22	0.22	Verschuieren 1983
Bioconcentration factor				
Log BCF	0.86 (calculated from water solubility)	0.85 (calculated from water solubility)	0.86 (calculated from water solubility)	Lyman et al. 1982
Explosive limits	No data	No data	4.3%-10.3%	OHM/TADS 1989

